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14. ABSTRACT
This grant provided support for a postdoc at the University of Michigan to assist in developing a grid-free particle method for electrostatic plasma simulations. The aim of the work is to substantially improve the accuracy and efficiency of these simulations. The proposed method is an alternative to traditional mesh-based methods such as particle-in-cell (PIC). In the new approach, the standard Eulerian formulation of the Vlasov-Poisson equation is replaced by a Lagrangian formulation in which the charge flow map is the key unknown quantity. Discretizing the Lagrangian formulation leads to a grid-free particle method. The investigators made progress in formulating and testing this approach. Numerical results are presented for the cold one-stream and two-stream instabilities. The method is especially well suited for tracking charge transport and resolving fine structures in phase space.

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Final Performance Report on AFOSR Grant FA9550-06-1-0529 (F016052) A Grid-Free Particle Method for Electrostatic Plasma Simulations

PI: Robert Krasny, Department of Mathematics, University of Michigan

August 27, 2007

This grant provided support for a postdoc, Lyudmyla Barannyk, at the University of Michigan, during the period September 1, 2006 - May 31, 2007, to assist in developing a grid-free particle method for electrostatic plasma simulations.

1 Objectives

This project is part of a larger effort funded by AFOSR (FA9550-05-1-0199, Major David Byers), in collaboration with Andrew Christlieb at Michigan State University, that aims to develop a grid-free particle method for plasma simulations. The majority of plasma simulations currently use the particle-in-cell (PIC) method [1, 2]. The advantage of PIC is that it uses a fast Poisson solver to obtain the electric field, but the results may exhibit mesh-induced effects such as artificial diffusion and anisotropy. In addition, geometrically complex domains present a problem for the fast Poisson solvers typically used in PIC.

The present work seeks to overcome these difficulties and substantially improve the accuracy and efficiency of plasma simulations for a wide range of applications. Our approach is based on the Lagrangian formulation of charged particle dynamics, in contrast to the standard Eulerian formulation in terms of the Vlasov-Poisson equation. The Lagrangian formulation leads naturally to a grid-free particle method. We incorporate several techniques from the study of vortex sheet motion in computational fluid dynamics [3].

2 Status of Effort

The investigators made progress in developing the Lagrangian formulation of charged particle dynamics, deriving a regularized system that satisfies charge neutrality and periodic boundary conditions, implementing an adaptive particle insertion scheme, and performing test computations. The work is being written up for publication [4]. The following section summarizes the approach and presents numerical results showing the method's capability.

3 Accomplishments/New Findings

Here we summarize the accomplishments and new findings obtained during the award period. Complete details are in an article being prepared for publication [4]. We start by recalling the standard Eulerian formulation of charged particle dynamics in terms of the Vlasov-Poisson equations.

3.1 Eulerian Formulation

Let $f(x,v,t)$ be the electron probability density function (pdf) in phase space, satisfying

$$f(x,v,t) \geq 0, \quad \int_{-\infty}^{\infty}\int_0^1 f(x,v,t)dxdv = 1, \tag{1}$$

where x is space (here 1D), v is velocity, and t is time. The pdf evolves by the Vlasov equation,

$$f_t + vf_x - Ef_v = 0, \tag{2}$$

where the electric field $E(x,t)$ is given by $E = -\phi_x$ and the potential function $\phi(x,t)$ satisfies the Poisson equation,

$$-\phi_{xx} = \rho, \tag{3}$$

with periodic boundary conditions. The charge density is

$$\rho(x,t) = -\int_{-\infty}^{\infty} f(x,v,t)dv + 1. \tag{4}$$

The Vlasov-Poisson equations (2-4) describe the evolution of the pdf $f(x,v,t)$. Next we describe an equivalent Lagrangian formulation.

3.2 Lagrangian Formulation

Consider the charge flow map,

$$\begin{pmatrix}\alpha\\ \beta\end{pmatrix} \to \begin{pmatrix}x(\alpha,\beta,t)\\ v(\alpha,\beta,t)\end{pmatrix}, \tag{5}$$

where (α,β) are Lagrangian parameters labeling a charged particle at location (x,v) in phase space at time t. This is shown schematically in Figure 1.
The equations defining the flow map are,

$$\begin{aligned} x_t(\alpha,\beta,t) &= v(\alpha,\beta,t), & (6)\\ v_t(\alpha,\beta,t) &= -\int_{-\infty}^{\infty}\int_0^1 (k(x(\alpha,\beta,t),x(\tilde{\alpha},\tilde{\beta},t)) + x(\tilde{\alpha},\tilde{\beta},t))\omega_0(\tilde{\alpha},\tilde{\beta})d\tilde{\alpha}d\tilde{\beta} \, + \, x(\alpha,\beta,t), & (7)\end{aligned}$$

where

$$k(x,y) = \frac{1}{2}\text{sign}(x-y) \tag{8}$$

is the electric field kernel and $\omega_0(\alpha,\beta)$ is the initial charge distribution. Equations (6-7) are simply Newton's equations in first order form. The integral on the right side of (7) gives the

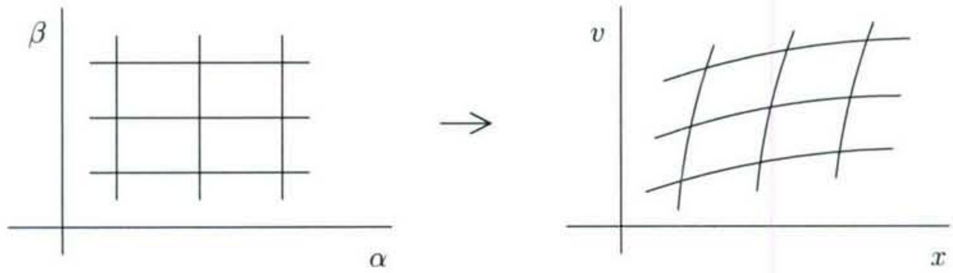


Figure 1: Charge flow map, (α, β): parameter space, (x, v): phase space.

electric field in terms of the flow map and initial charge distribution. We assume here that the spatial domain is 1D and the solution is periodic with period $L = 1$, but these are not essential restrictions. Equations (6-8) are the desired Lagrangian formulation for charged particle dynamics in phase space.

3.3 Particle Discretization

We consider a cold stream in which the charge is supported on a curve in phase space, so that the flow map reduces to the form $x(\alpha, t), v(\alpha, t)$. We use the midpoint rule to discretize the electric field integral in (7). Then $\alpha_i = (i - \frac{1}{2})/N, i = 1 : N$ are the discretization points in parameter space and $(x_i(t), v_i(t)) = (x(\alpha_i, t), v(\alpha_i, t))$ are the corresponding particles in phase space. The discrete evolution equations are

$$x_i' = v_i, \tag{9}$$

$$v_i' = -\sum_{j=1}^{N}(k(x_i, x_j) + x_j)\, w_j \;+\; x_i, \tag{10}$$

where $w_j = 1/N$ are the quadrature weights. The discontinuity in the kernel is handled by setting $k(x, x) = 0$. The 4th order Runge-Kutta method is used for timestepping.

Figure 2 shows the numerical results for a perturbed uniform stream with $N = 50, \Delta t = 0.004$. The solution is plotted over two periods, $0 \leq x \leq 2$. Two types of particles are plotted, active (red) and passive (blue). The active particles, (x_i, v_i), carry charge and contribute to the sum defining the electric field. The passive particles have Lagrangian parameter values at the endpoints of the intervals in parameter space. The passive particles are used in the adaptive particle insertion scheme, described below.

The stream rolls up into a vortex in phase space. The vortex is associated with particle trapping as particles cycle back and forth in the given period. Other particles escape and are advected into neighboring periods, leading to the formation of long thin filaments in the stream. The simulation loses accuracy as time proceeds, as shown by the self-intersection of the stream at late times. Simply using a smaller time step Δt and a larger number of particles N is not a practical way of maintaining resolution. Moreover, as shown in Figure 3a, even as the computation is refined, the inner portion of the spiral is tangled. We believe this tangling is due to a singularity in the exact solution. To address these issues we employ regularization and adaptive particle insertion, as explained in the next two sections.

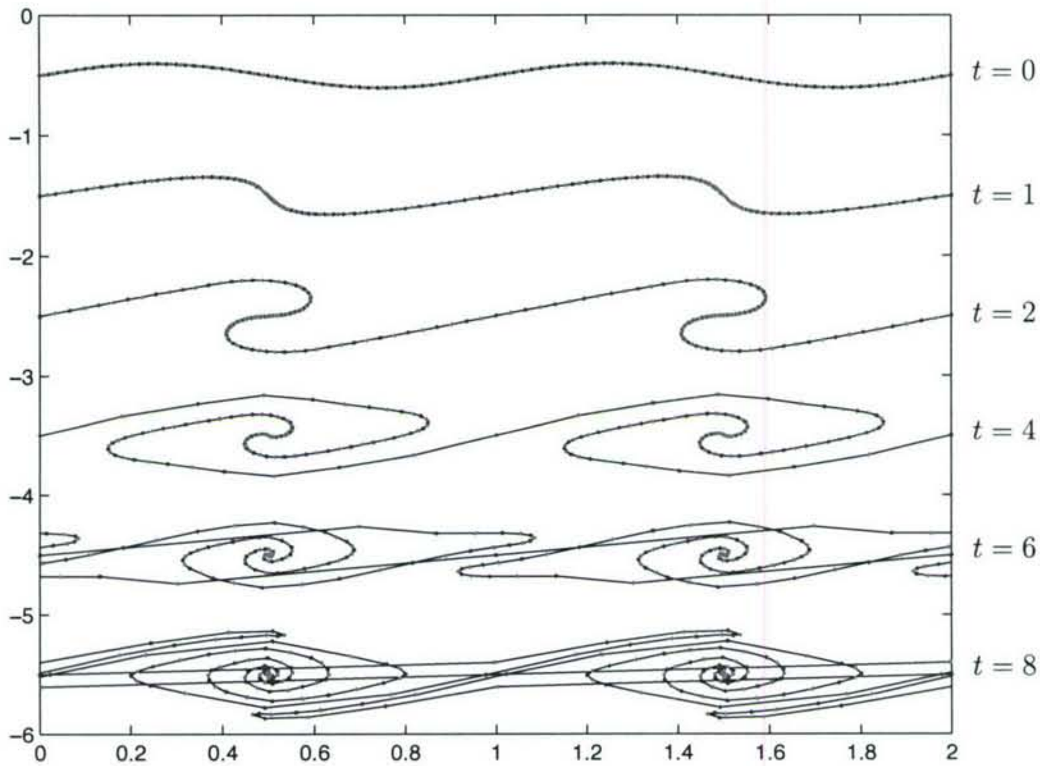


Figure 2: Cold stream, $N = 50$, $\Delta t = 0.004$, active particles (red), passive particles (blue).

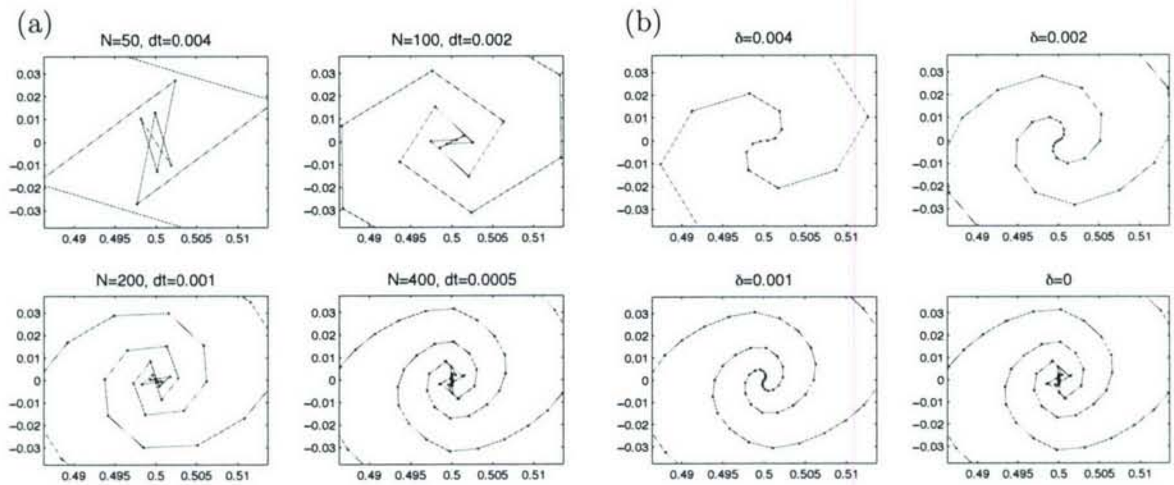


Figure 3: Cold stream, closeup of spiral core at $t = 8$. (a) The solution converges slowly as N increases and Δt decreases. The inner portion of the spiral remains tangled. (b) The regularized solutions with $\delta > 0$ roll up smoothly and are free of tangling.

3.4 Regularization

Consider the following regularized approximation of the electric field kernel,

$$k_\delta(x,y) = \frac{1}{2}\frac{x-y}{((x-y)^2+\delta^2)^{1/2}}, \tag{11}$$

where $\delta > 0$ is a smoothing parameter. The exact kernel, in equation (8), is recovered in the limit $\delta \to 0$. Using the regularized kernel we obtain a regularized system,

$$x_t(\alpha,t) = v(\alpha,t), \tag{12}$$

$$v_t(\alpha,t) = -\int_{-\infty}^{\infty}\int_0^1 k_\delta(x(\alpha,t),x(\tilde{\alpha},t))\omega_0(\tilde{\alpha})d\tilde{\alpha} + \overline{\rho}\int_0^1 k_\delta(x(\alpha,t),y)dy - a, \tag{13}$$

where the constants $\overline{\rho}$ and a are chosen to enforce charge neutrality and periodicity [4]. Using the midpoint rule as before, we obtain a particle discretization of the regularized system. As shown in Figure 3b, the solution of the regularized system is free of tangling for $\delta > 0$. But there is still a need for adaptive particle insertion to maintain resolution without using prohibitively large N.

3.5 Adaptive Particle Insertion

To maintain resolution as the curve evolves, we adaptively insert new particles at each time step [3]. Figure 4 defines two quantities, (a) d_1: chord length of the interval, (b) d_2: distance from the active particle to the chord. If either of these quantities is larger than a user-specific value, the interval is split, as depicted in Figure 4c. After an interval is split, the quadrature weights are reset.

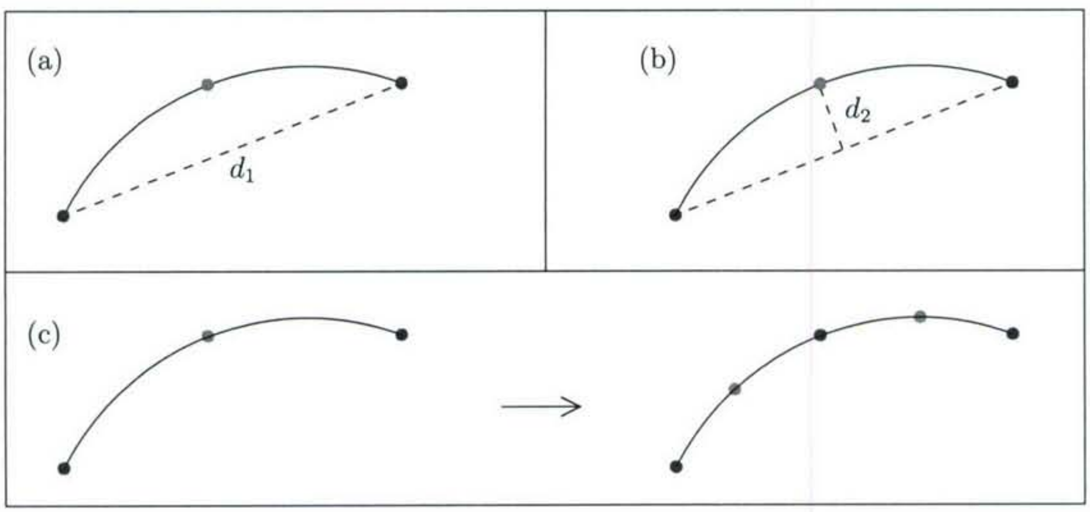


Figure 4: Adaptive particle insertion. (a) d_1: chord length, (b) d_2: particle-chord distance, (c) panel splitting; the active particle becomes passive and two new passive particles are inserted using quadratic interpolation with respect to the Lagrangian parameter.

3.6 Numerical Results

Figure 5a shows a simulation of the regularized system (11-13) with $\delta = 0.1$ and adaptive particle insertion. The initial number of particles is $N = 400$ and the final number is $N = 2920$. To clarify the charge transport in phase space, the charge coming from each initial period is colored (e.g. blue: $0 \leq x \leq 1$, red: $1 \leq x \leq 2$, etc.). The closeup in Figure 5b shows that the fine scale structures are well-resolved and free of tangling. The results suggest the presence of chaotic dynamics due to a heteroclinic tangle.

Figure 6 shows a preliminary simulation of the cold two-stream instability. In this case there are two streams of particles moving in opposite directions. The initial charge density was perturbed. The streams roll up smoothly into a vortex in phase space. This is a step towards extending the code to handle warm charge distributions.

3.7 Ongoing Work

(a) We're performing various checks of the numerical accuracy, e.g. energy conservation, time integration (for $\delta = 0$ and $\delta > 0$).

(b) We believe that a cusp singularity forms at a finite time in the charge distribution and electric field as a function of the spatial x-coordinate. We will document this numerically using spectral analysis (FFT).

(c) We're studying the phenomenon of particle trapping. The aim is to determine how much of the charge remains trapped in its original period, how much is advected and trapped in neighboring periods, and how much undergoes free streaming. Charge transport is a fundamental issue and the present approach may well provide new insights.

(d) The code is being extended to handle warm distributions, i.e. those in which the charge is distributed over a region in phase space, as opposed to simply a curve or a finite set of curves. This will enable us to study Landau damping and compare with previous results.

(e) We intend to perform a detailed comparison with PIC simulations.

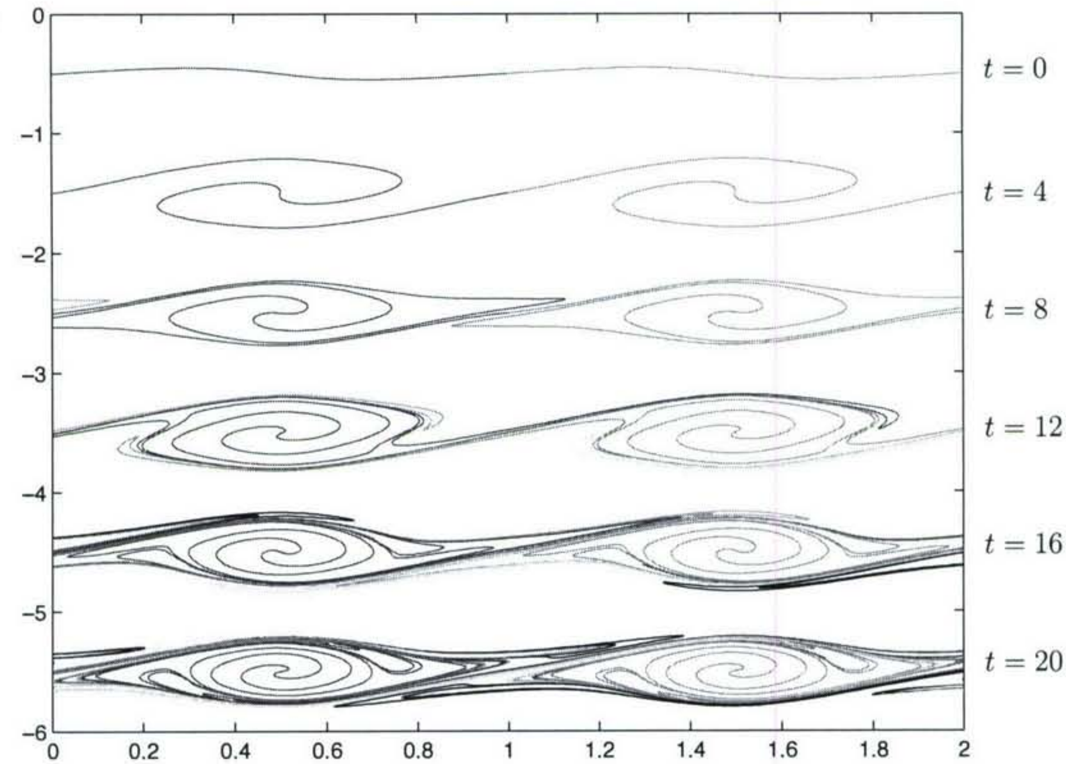
3.8 Summary

The results presented in the previous sections demonstrate the capability of the grid-free particle approach under development. The method is especially well suited for studying charge transport and filamentation. We believe this approach will substantially improve the accuracy and efficiency of plasma simulations for a wide range of applications.

4 Personnel Supported

The project provided 50% support for a postdoc, Lyudmyla Barannyk. Dr. Barannyk is starting a tenure-track position at the University of Idaho in August, 2007. The project extends the work started last summer by Benjamin Sonday when he was an undergraduate. Mr. Sonday is currently a graduate student at Princeton University with support from a Department of Energy Computational Science Graduate Fellowship.

(a)



(b)

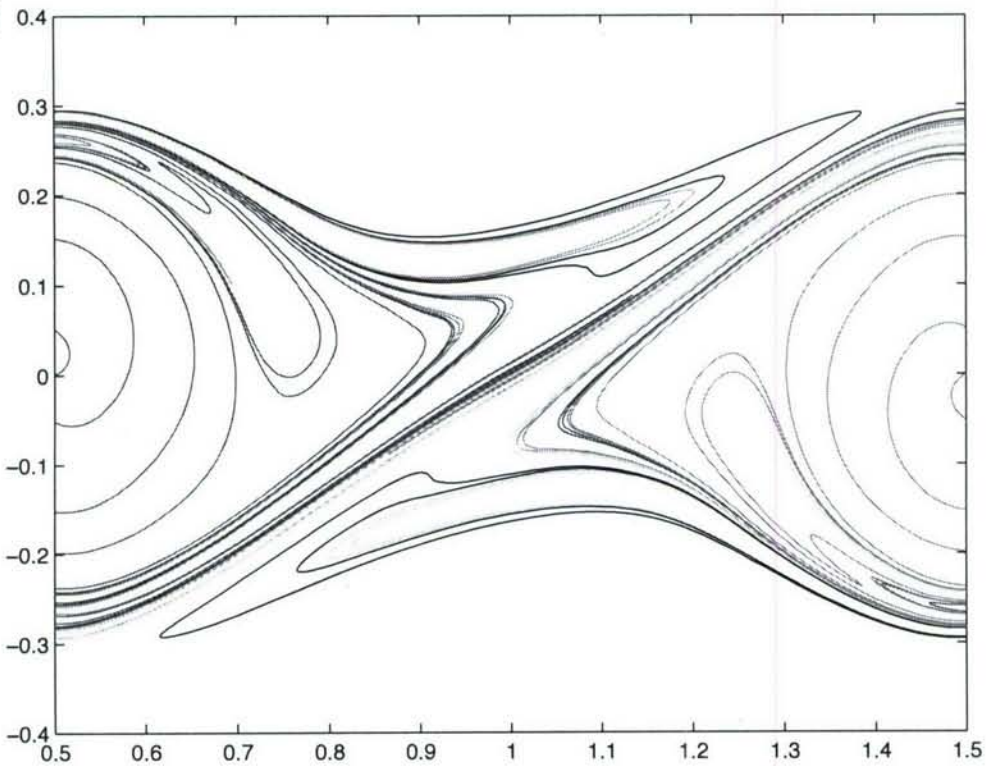


Figure 5: Cold stream, long time evolution, regularized ($\delta = 0.1$), adaptive particle insertion. Charge coming from each initial period is colored, e.g. blue: $0 \leq x \leq 1$, red: $1 \leq x \leq 2$, etc. (a) time: $0 \leq t \leq 20$, initial $N = 400$, final $N = 2920$, (b) closeup at $t = 20$.

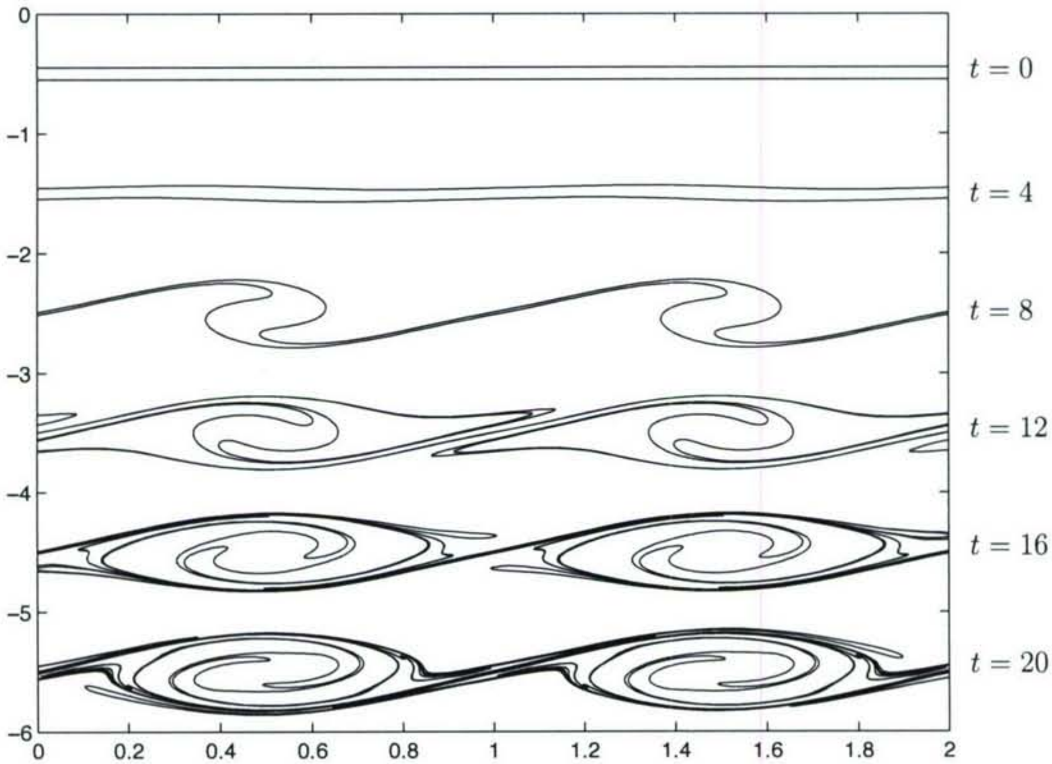


Figure 6: Cold two-stream instability.

5 Publications

The work accomplished during the support period is being prepared for publication [4]. The article will be sent to the program manager, Dr. Fariba Fahroo, upon completion. The group has published several previous articles with AF support [5–7].

6 Interactions/Transitions

The work supported by this award was presented at three conferences.

- American Physical Society, Division of Plasma Physics, Philadelphia, November, 2006
- Society for Industrial and Applied Mathematics, Conference on Computational Science and Engineering, Costa Mesa, February, 2007
- International Congress on Industrial and Applied Mathematics, Zurich, July, 2007

It will also be presented at the upcoming APS meeting of the Division of Plasma Physics, Orlando, November, 2007. The project is part of a larger effort supported by AFOSR (FA9550-05-1-0199, Major David Byers) in collaboration with Andrew Christlieb at Michigan State University.

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